

Atom Resonance Lines for Modeling Atmosphere
NASA Grant NAG5-12751

Annual Report #2

For the period 15 January 2004 through 14 January 2005

Principal Investigator
Kate P. Kirby

January 2005

Prepared for
National Aeronautics and Space Administration
Washington, DC 20546

SMITHSONIAN INSTITUTION
ASTROPHYSICAL OBSERVATORY
CAMBRIDGE, MASSACHUSETTS 02138

Director: Charles Alcock

The Smithsonian Astrophysical Observatory
is a member of the
Harvard-Smithsonian Center for Astrophysics

The NASA Technical Officer for this grant is Hashima Hasan,
NASA Headquarters, Code SZ, Washington, DC 20546 202-358-0743

Studies of Pressure-broadening of Alkali Atom Resonance Lines for Modeling Atmospheres of Extrasolar Giant Planets and Brown Dwarfs

Grant NAG5-12751

Principal Investigator: K. Kirby

Co-Principal Investigators: J. Babb and K. Yoshino

Progress report for the period 01/15/2004 through 01/14/2005

We report on progress made in a joint program of theoretical and experimental research to study the line-broadening of alkali atom resonance lines due to collisions with species such as helium and molecular hydrogen. Accurate knowledge of the line profiles of Na and K as a function of temperature and pressure will allow such lines to serve as valuable diagnostics of the atmospheres of brown dwarfs and extra-solar giant planets.

A new experimental apparatus has been designed, built and tested over the past year, and we are poised to begin collecting data on the first system of interest, the potassium resonance lines perturbed by collisions with helium.

On the theoretical front, calculations of line-broadening due to sodium collisions with helium are nearly complete, using accurate molecular potential energy curves and transition moments just recently computed for this system. In addition we have completed calculations of the three relevant potential energy curves and associated transition moments for K - He, using the MOLPRO quantum chemistry codes. Currently, calculations of the potential surfaces describing K-H₂ are in progress.

1. Theoretical Progress

A graduate student, Mr. Cheng Zhu, has developed an efficient suite of computer codes to calculate atomic line-broadening due to collisions with atom perturbers. Test calculations for Li colliding with He were performed, and a manuscript describing this work, "Theoretical study of pressure broadening of lithium resonance lines by helium atoms" (Zhu, Babb, and Dalgarno, 2005) has been submitted to Physical Review A. This research was also presented as a poster paper at the American Physical Society Division of Atomic, Molecular, and Optical Physics (DAMOP) annual meeting (Tucson, AZ) in May 2004 (Zhu, Babb, and Dalgarno, 2004).

As described in last year's Progress Report, Mr. Cheng Zhu has also carried out calculations of the dynamic polarizabilities of Na, K, and Rb and their long-range interaction with He. A paper on this work, "Dipole polarizabilities of excited alkali-metal atoms and long-range interactions of ground- and excited-state alkali-metal atoms with helium atoms" was published in 2004 (Zhu *et al.*, 2004).

Using accurate potential energy curves and transition dipole moments for Na-He, Zhu, Babb and Dalgarno have carried out quantum mechanical calculations of the emission and absorption profiles of the sodium $3s - 3p$ resonance lines under the influence of a perturbing gas of helium. Emission and absorption coefficients have been obtained for temperatures ranging between 158 K and 3000 K, and at wavelengths between 500 and 760 nm. This work will be reported on as a poster paper at the 2005 DAMOP meeting (Lincoln, NE) in May.

Accurate calculations of the potential energy curves and transition dipole moments for K-He have just been completed, using the MOLPRO quantum chemistry codes. A Multi-Reference Configuration Interaction (MRCI) method was implemented to obtain the molecular data, which will then be used to calculate the collision-broadening.

At present, we are working on calculating the potential surfaces for K ($4s, 4p$) interacting with molecular hydrogen. These have been obtained for fixed H_2 internuclear separation at a range of collision angles, with respect to the molecular axis. We will also allow for variation of the molecular hydrogen bond length. These calculations are considerably more complex and time-consuming than the atom-atom calculations.

In September 2004, at the Star and Planet Formation Internal Symposium held at the Harvard-Smithsonian Center for Astrophysics, Dr. James Babb gave a talk on the work funded by this NASA grant, titled: "Theoretical and experimental studies of pressure broadened alkali metal atom resonance lines for modeling brown dwarf spectra." The powerpoint version of the talk is available at the conference website, <http://cfa-www.harvard.edu/spfis> (Babb, 2004).

2. Experimental Progress

The experimental apparatus described last year has now been realized and measurements of the line broadening of potassium due to collision with helium are about to be collected.

To reproduce the conditions of the environments we want to study, the apparatus was designed to allow measurements at different buffer gas pressures (ranging from a few hundred torr to atmospheric pressure) and high temperature (about 900 K). The cell was fabricated according to the design shown in Figure 1. The cell body is composed of three welded tubes of grade 330 stainless steel, chosen for its resistance to the corrosive effects of alkali-metal gases at high temperature. The middle tube is the gas chamber and it is closed by MgO windows sealed with graphite gaskets. The end tubes on each side of the gas chamber contain a cylinder and a spring to push down the MgO windows onto the gas chamber, thereby allowing the buffer gas pressure in the chamber to reach values as high as atmospheric pressure. The end tubes are closed by quartz windows sealed with Viton O-rings. All the cell body tubes are independently connected to a vacuum line.

The potassium sample is placed in a 330 grade stainless steel reservoir attached to the cell by a Swagelok fitting allowing the reservoir to be removed readily for sample

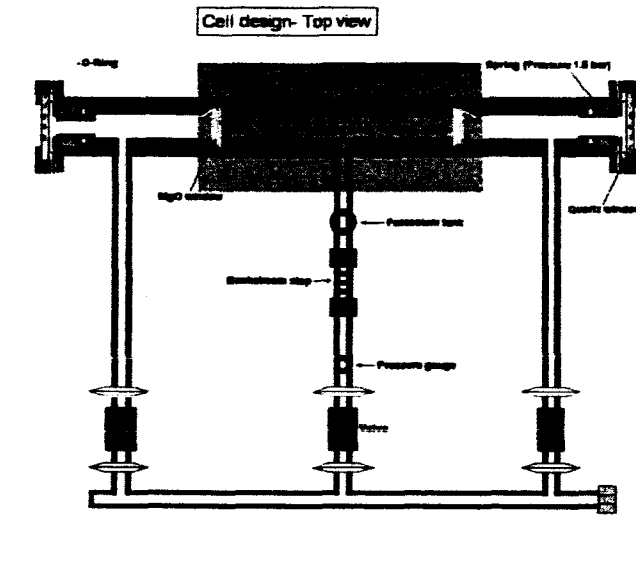


Figure 1: Cell design.

replacement. The sample is heated in the reservoir by homemade heaters. The temperatures of the reservoir and of the tube leading to the gas chamber are regulated through a commercial temperature controller. The gas chamber is inserted in a specially designed split tube furnace that fits within our experimental size constraints. The oven ensures that there is a uniform temperature along the path-length of the gas chamber and is built to facilitate the removal of the cell from the apparatus.

In order to improve the wavelength accuracy and the reproducibility of the measurements as required for the eventual comparison of the data with calculations we had to change the spectrometer driving system. A new scan controller and motor were acquired at no cost to NASA using Smithsonian Institution internal funds. Homemade software was written to allow a PC workstation to centrally control the scan controller, the shutters in the interferometer arms, and the acquisition of spectra from the CCD camera. We also upgraded our vacuum pump station and ordered a more stable and powerful infrared light source, both at no cost to NASA using internal Smithsonian Institution funds.

A key feature of the experiment is the utilization of a Mach-Zehnder interferometer to create hook-like fringes, from which the absolute atom number density of potassium can be determined. Figure 2 shows those fringes distorted by the potassium line observed at 766.49 nm. The ensemble was also fixed on an optical table, obtained at no cost to NASA, to avoid any perturbations caused by the room vibrations. A poster paper on the apparatus design, "Visible-IR experiment for absolute spectroscopic measurements

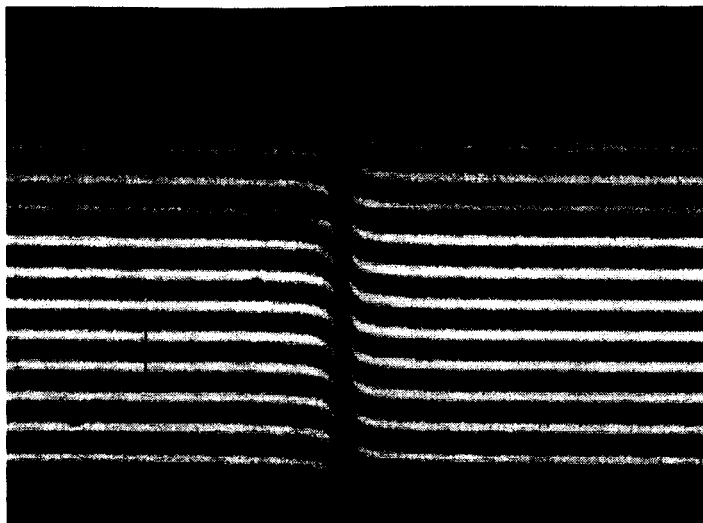


Figure 2: Potassium line observed at 766.49 nm on the spectrometer CCD.

of alkali vapors," was given at the American Physical Society Division of Atomic, Molecular, and Optical Physics (DAMOP) annual meeting (Tucson, AZ) in May 2004 (Shindo et al., 2004). An abstract for a poster paper describing the first measurements on K-He line broadening has been submitted to the 2005 DAMOP meeting (Lincoln, NE).

References

- J. Babb, http://cfa-www.harvard.edu/spfisppt/babb_j.ppt, (2004).
- F. Shindo, J. Babb, K. Kirby, and K. Yoshino, *Bull. Am. Phys. Soc.* **49**, 25 (2004).
- C. Zhu, J. Babb, and A. Dalgarno, *Bull. Am. Phys. Soc.* **49**, 25 (2004).
- C. Zhu, J. Babb, and A. Dalgarno, submitted to *Phys. Rev. A* (2005).
- C. Zhu, A. Dalgarno, S. Porsev, and A. Derevianko, *Phys. Rev. A* **70**, 032722 (2004).